(no nucleotide, ATP, transition state, and ADP). Initial *in silico* work focused on resolving differences between high- and low-resolution experimentally determined structures through the use of the molecular dynamics flexible fitting (MDFF) method. From these simulations, unrestrained all-atom, long time scale molecular dynamics simulations were performed on each state. Results show important differences in structure and dynamics of the protein in each hydrolysis state and assist in characterization of the p97 hydrolysis pathway.

**2929-Pos**
**CHARMM-GUI: Brining Advanced Computational Techniques to Web Interface**
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CHARMM-GUI, http://www.charmm-gui.org, has been developed to provide a web-based graphical user interface to generate various input files and molecular systems to facilitate and standardize the usage of common and advanced simulation techniques in CHARMM. We have made a significant amount of efforts to implement basic and common molecular dynamics simulation techniques into web interface and the web interface has generated a multitude of positive feedback from our users. In this work, we describe our latest efforts to bringing more advanced molecular modeling and simulation techniques to the web interface, such as membrane system building with more lipid types, ligand binding free energy calculation, electron microscopy density map fitting, protein-protein docking, transition path finding and free energy along the path, and NMR structure calculation.

**2930-Pos**
**Molecular Mechanisms How Mercury Inhibits Water Permeation of Aquaporin-1: Understanding by Molecular Dynamics Simulation**
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Aquaporin (AQP) functions as a water-conducting pore. Mercury inhibits the water permeation through AQP. Although site-directed mutagenesis has revealed that mercury binds to Cys189 during the inhibition process, it is not fully understood how this inhibits the water permeation through AQP1. Here, we performed 40 ns molecular dynamics simulations of bovine AQP1 with mercury (Hg-AQP1) or without mercury (Free AQP1). In Hg-AQP1, Cys191 (Cys189 in human AQP1) is converted to Cys-$SHg^+$ in each monomer. During each last 10 ns, we observed water permeation events occurred 23 times in Free AQP1 and never in Hg-AQP1. Mercury binding did not influence the whole structure, but did induce a collapse in the orientation of several residues at the ar/R region. In Free AQP1, backbone oxygen atoms of Gly190, Cys191, and Gly192 lined, and were oriented to, the surface of the water pore channel. In Hg-AQP1, however, the $SHg^+$ of Cys191-$SHg^+$ was oriented towards the outside of the water pore. As a result, the backbone oxygen atoms of Gly190, Cys191, and Gly192 became disorganized and the ar/R region collapsed, thereby obstructing the permeation of water. We conclude that mercury disrupts the water pore of AQP1 through local conformational changes in the ar/R region.

**2931-Pos**
**Molecular Dynamics Studies of the ERK2 Tyrosine Kinase**
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The extracellular-regulated kinase (ERK) belongs to a class of mitogen activated protein kinases (MAPKs) which respond to growth signals in the environment and regulate cell growth and division. Consequently, these signal pathways are often implicated in various cancers and growth diseases. Using molecular dynamics simulations, we studied the ERK protein in various stages of activation. By studying the quasiharmonic modes, correlation maps, and information flow in the system, we developed a coherent picture of the structural and dynamic changes upon activation of the protein.

**2932-Pos**
**The Effect of Genetic Mutations on Structural and Mechanical Properties of Collagen: Molecular Dynamics Simulations**
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Osteogenesis Imperfecta is a disease characterized by too little collagen in the body, causing brittle bones, permanent disfigurement, and often death. To provide fundamental understanding of the molecular basis of these diseases, extensive molecular dynamics simulations were conducted using the AMBER 10.0 suite. A Glycine-Proline-Hydroxyproline tropocollagen molecule was used as a building block for a fibril. The central tropocollagen molecule was later modified to corresponding mutations. Electrostatic measurements, hydration and ion patterns were determined, garnering an observation of a hydrophobic dipole. Our simulations indicate that the mutations significantly affect binding and mechanical properties of the collagen fibrils. Moreover, we predict that the high death rate related to lysine mutation can be explained by the increase in diameter and significant loss of mechanical properties in collagen fibril.

**2933-Pos**
**Mechanism of Glycan Receptor Recognition and Specificity Switch for Avian, Swine and Human Adapted Influenza Virus Hemagglutinins: A Molecular Dynamics Perspective**
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Hemagglutinins (HA's) from duck, swine and human influenza viruses have previously been shown to prefer avian and human glycan receptor analogues with distinct topological profiles, pentasaccharides LSTa ($\alpha$-2,3 linkage) and LSTc ($\alpha$-2,6 linkage), in comparative molecular dynamics studies. Based upon detailed analyses of the dynamic motions of the receptor binding domains (RBD's) and interaction energy profiles with individual glycan residues, we have identified approximately 30 residue positions and secondary structural elements (SSE's) in the RBD that present distinct profiles with the receptor analogues. Glycan binding constrained the conformational space sampling by the HA. Electrostatic steering appeared to play a key role in glycan binding specificity. The complex dynamic behaviors of the major SSE and trimeric interfaces with or without bound glycans suggested that networks of interactions might account for species specificity in these low affinity and high avidity (multivalent) interactions between different HA and glycans. Contact frequency, energetic decomposition and H-bond analyses revealed species-specific differences in HA-glycan interaction profiles, not readily discernable from crystal structures alone. Interaction energy profiles indicated that mutation events at the set of residues such as 145, 156, 158 and 222 would favor human or avian receptor analogues, often through interactions with distal asialo-residues. These results correlate well with existing experimental evidence, and suggest new opportunities for simulation-based vaccine and drug development.

**2934-Pos**
**Study of Interactions Between Neuron-Specific Enolase and B-Type Phosphoglycerate Mutase with Molecular Dynamics Simulations**
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Molecular dynamics simulations were used to examine the interaction of human B-type phosphoglycerate mutase (dPGM-B) and neuron-specific enolase (NSE). Specifically, we studied the interactions of 31 orientations of these enzymes by means of the effective energy function (EEF1) implicit solvation method available in program CHARMM. Interactions of the enzymes were grouped into five different NSE - dPGM-B complexes. Interactions between active regions of the enzymes occurred preferentially as in three of the five groups the enzymes interacted with their active regions. With periodically increased temperature dynamics the close conformation of dPGM-B was obtained as the C-terminal tail capped the active pocket in the presence of the 2-phosphoglycerate (2PG) substrate. Cleavage of 2PG through the residue loop Trp16-Gly24 was observed for a separate subunit of dPGM-B. Preferential interaction between active regions of the enzymes implicitly implies tendency of direct transfer of 2PG (channeling) between dPGM-B and NSE. Such phenomenon, however, needs additional study as interaction of the active regions of the enzymes might bring delays into conformation changes of dPGM-B which are necessary for proper direction of 2PG to the surface of the enzyme and consequent cleavage.

**2935-Pos**
**Recognition and Signaling in DNA Mismatch Repair: Interdomain Communication in T. Aquaticus Muts Proteins**
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Allosteric communication events involving multifaceted protein architectures are critical in complex biological processes, including DNA mismatch repair (MMR). MutS and its homologs, highly conserved proteins in both prokaryotes and eukaryotes, initiate MMR by recognizing mispaired DNA and signaling downstream repair. DNA binding is allosterically coupled to ATPase activity at the nucleotide binding sites ~70 Å away. Modern theories on allosteric